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14. ABSTRACT

Optimally designed composite materials offer the best material systems to achieve the many demands that are being placed on structures and components in Air Force applications. We have adapted the topology optimization method to design three-dimensional composite microstructures with multifunctional characteristics. These include optimal multifunctional materials with optimal electrical conductivity, thermal conductivity, elastic moduli, dielectric constant, and fluid permeability.
In many instances, the optimal microstructures were entirely new, and in all instances the designed materials are manufacturable.

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1 Introduction

Increasingly, a variety of performance demands are being placed on material systems. In Air Force applications these requirements include component structures that have desirable mechanical, thermal, electrical, optical, acoustic and flow properties, and low weight. Clearly, the structure should be able to carry mechanical loads. Desirable thermal properties include high thermal conductivity to dissipate heat and thermal expansion characteristics that match the attached components. In the case of porous cellular solids, heat dissipation can be improved by forced convection through the material, but in these instances the fluid permeability of the porous material must be large enough to minimize power requirements for convection. Desirable optical and acoustic properties include materials that can control the propagation of light and sound waves through them, respectively. It is difficult to find single homogeneous materials that possesses these multifunctional characteristics.

Composite materials are ideally suited to achieve multifunctionality since the best features of different materials can be combined to form a new material that has a broad spectrum of desired properties [1, 2]. However, a systematic means of designing composite materials with multifunctional characteristics has been lacking. These materials may simultaneously perform as ultralight load-bearing structures, enable thermal and/or electrical management, ameliorate crash or blast damage, and have desirable optical and acoustic characteristics. The purpose of this project is to take the first steps to fill this gap using optimization techniques.

It is desired to design a composite material with N different effective properties or responses, which we denote by $K_e^{(1)}, K_e^{(2)}, \ldots, K_e^{(N)}$, given the individual properties of the phases. In principle, we would like to know the region (set) in the multidimensional space of effective properties in which all composites must lie (see Fig. 1 for a two-dimensional illustration). The size and shape of this region depends on how much information about the microstructure is specified and on the prescribed phase properties. For example, if not even the volume fractions are not specified, this set is clearly larger than the one in which the the volume fractions are specified. The determination of the allowable region is generally a highly complex problem. However, the identification of the allowable region can be greatly facilitated if *cross-property* bounds on the effective properties can be found. Cross-property bounds are inequalities that rigorously link different effective properties to one another, even when their respective governing equations are uncoupled (e.g., between conductivity and elastic moduli [3, 4]). When cross-property bounds are optimal (i.e., the best possible bounds), they can be used to identify the boundary of the allowable region. Numerical optimization methods, such as the topology optimization technique [5, 6], can then be used to find specific microstructures that lie on the boundary. Despite its importance to multifunctional design of composites, cross-property relations have yet to applied for this purpose.

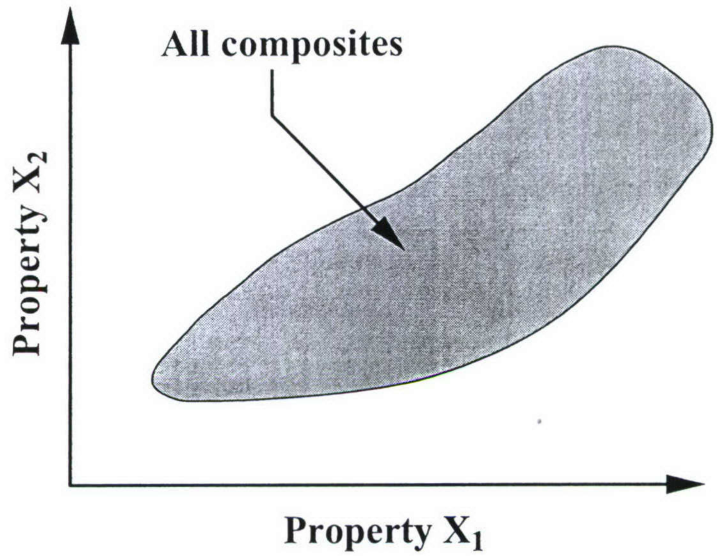

Figure 1: Schematic illustrating the allowable region in which all composites with specified phase properties must lie for the case of two different effective properties.

2 Accomplishments

We have adapted the topology optimization method to design three-dimensional composite microstructures with multifunctional characteristics [7–9, 11]. We have recently shown that triply periodic two-phase bicontinuous composites with interfaces that are the Schwartz P and D minimal surfaces are not only geometrically extremal but extremal for simultaneous transport of heat and electricity [7, 8]. Figure 2 depicts the Schwartz P and D structures. Triply periodic minimal surfaces are objects of great interest to physical scientists, biologists, and mathematicians. They arise in a variety of systems: block copolymers, nanocomposites, micellar materials, and lipid bilayers, and other biological formations. The multifunctionality of the Schwartz P and D minimal surfaces has been further established by demonstrating that they are also extremal when a competition is set up between the effective bulk modulus and electrical (or thermal) conductivity of the bicontinuous composite [9]. It is important to note that current self-assembly techniques enable one to manufacture three-dimensional composites whose interfaces are triply periodic minimal surfaces [10].

Many questions concerning the aforementioned minimal surfaces remain. What are optimal structures when $\phi_1 \neq 1/2$? Do optimal bicontinuous structures possess surfaces of *constant mean curvature*? Are these bicontinuous structures optimal in any other sense? For example, in the case in which one of these phases is a fluid (i.e., porous-medium case), with specified porosity and specific surface, is the Stokes-flow *fluid permeability* k extremal? We have recently computed the fluid permeabilities of these and other triply periodic bicontinuous structures at a porosity $\phi = 1/2$ using the immersed boundary finite volume method [11]. The other triply periodic porous media that we studied include the Schoen gyroid minimal surface,

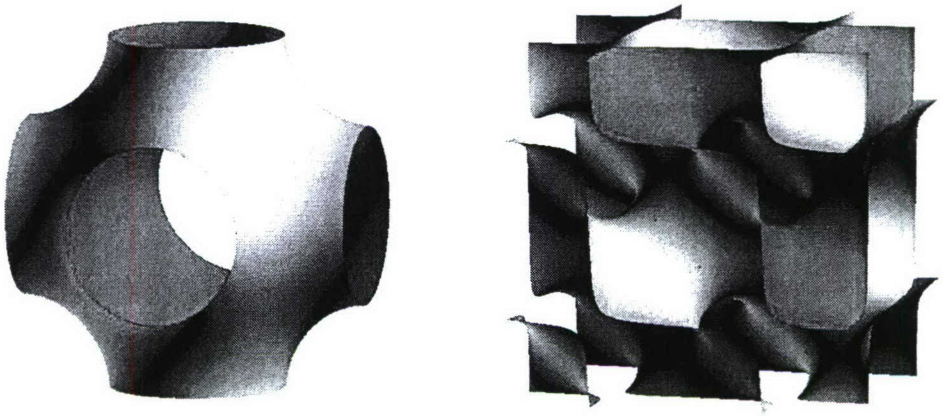

Figure 2: Unit cells of two different minimal surfaces with a resolution of $64 \times 64 \times 64$. Left panel: Schwartz simple cubic surface. Right panel: Schwartz diamond surface.

two different pore-channel models, and an array of spherical obstacles arranged on the sites of a simple cubic lattice. Our computed fluid permeabilities for the three minimal surfaces are summarized in Table 1 along with corresponding results for the circular and square channels with minimal pores and the simple cubic array of spherical obstacles at the porosity $\phi = 1/2$. We find that the Schwartz P porous medium indeed has the largest fluid permeability among all of the six triply periodic porous media considered in this paper. The fluid permeabilities are shown to be inversely proportional to the corresponding specific surfaces for these structures. This leads to the conjecture that the maximal fluid permeability for a triply periodic porous medium with a simply connected pore space at a porosity $\phi = 1/2$ is achieved by the structure that globally minimizes the specific surface.

Table 1: The fluid permeability k and specific surface s at $\phi = 1/2$ for six different triply periodic porous media models. The pore-channel results are presented for the minimal pore case ($b = 0$). SC and BCC stand for simple cubic and body centered cubic lattices, respectively.

Model	k	s	Symmetry
Schwartz P surface	3.4765×10^{-3}	2.3705	SC
Circular channel/spherical pore	3.4596×10^{-3}	2.6399	SC
Square channel/cubic pore	3.0743×10^{-3}	3.0000	SC
Spherical obstacle	3.0591×10^{-3}	3.0780	SC
Schoen G surface	2.2889×10^{-3}	3.1284	BCC
Schwartz D surface	1.4397×10^{-3}	3.9011	SC

In another work, we studied triply-periodic surfaces with minimal surface area under a constraint in the volume fraction of the regions (phases) that the surface separates [12]. Using a variational level set method formulation, we presented a theoretical characterization of and a numerical algorithm for computing these surfaces. We used our theoretical and computational formulation to study the optimality of the Schwartz primitive (P), Schwartz diamond (D), and Schoen gyroid (G) surfaces when the volume fractions of the two phases are equal and explore the properties of optimal structures when the volume fractions of the two phases are not equal. We showed that the P, D and G surfaces are all local optima of the surface area for equal volume fractions and are actually local minima of the total surface area, with P providing the smallest surface area. At non-equal volume fractions, we found optimal surfaces with non-zero mean curvature.

Interestingly, we have recently shown that the Schwartz P minimal surface appears to maximize the mean survival time τ (or, equivalently, minimize the reaction rate τ^{-1}) for diffusion-controlled reactions [13]. Diffusion occurs in the trap-free (or pore) region of a two-phase material. A diffusing particle is absorbed whenever it comes in contact with the pore–trap interface. To summarize, we have shown that two-phase material with interfaces that are certain minimal surfaces are optimized in a multifunctional sense, i.e., thermal/electrical competition, moduli/conductivity competition, fluid permeability, and mean survival time.

The drive toward increased semiconductor device densities and improved performance has set in motion the search for low dielectric constant materials. While introducing porosity in silica holds promise for reducing the dielectric constant, it remains elusive how to accomplish this without seriously degrading the thermo-mechanical performance. Applying rigorous cross-property relations, we identified the extremal porous material structure that possesses the desired reduction in dielectric constant while providing the highest possible stiffness for any given level of porosity [14]. The optimal microstructures turn out to be certain multiscale porous media. We show that spherical voids arranged on the sites of Bravais lattices (FCC and BCC structures) provide excellent approximations to the optimal structures. Figure 3 compares the performance of the optimal multiscale structure to the case of identical spherical voids arranged on the sites of the FCC lattice. This structural design is crucial to the integration of porous low-dielectric materials into microelectronics and should serve as a guide to future synthetic efforts. Using recently developed self-assembly techniques, we also demonstrate that structures approaching the optimal one can be fabricated.

More recently, we have considered multifunctional optimization for the design of two-dimensional two-phase composites [15]. This includes competition between effective electrical and thermal conductivities, effective bulk modulus and thermal conductivity and effective shear modulus and thermal conductivity.

We reported modulus/density scaling relationships for cubic (C), hexagonal (H) and worm-like disordered (D) nanoporous silicas prepared by surfactant-directed self-assembly [16] Over the relative density range, 0.5 to 0.65, Young's modulus scales as $(density)^n$ where $n_{(C)} < n_{(H)} < n_{(D)} < 2$, indicating that nanostructured porous silicas exhibit a structure-specific hierarchy of modulus values $D < H < C$. Scaling exponents less than 2 emphasize that the moduli are less sensitive to porosity than those of natural cellular solids, which possess extremal moduli based on linear elasticity theory.

We are only in the infancy of designing multifunctional via optimization techniques, but our preliminary results together with advances in fabrication methods suggest that this approach holds great promise to create the next generation materials. Many other functions

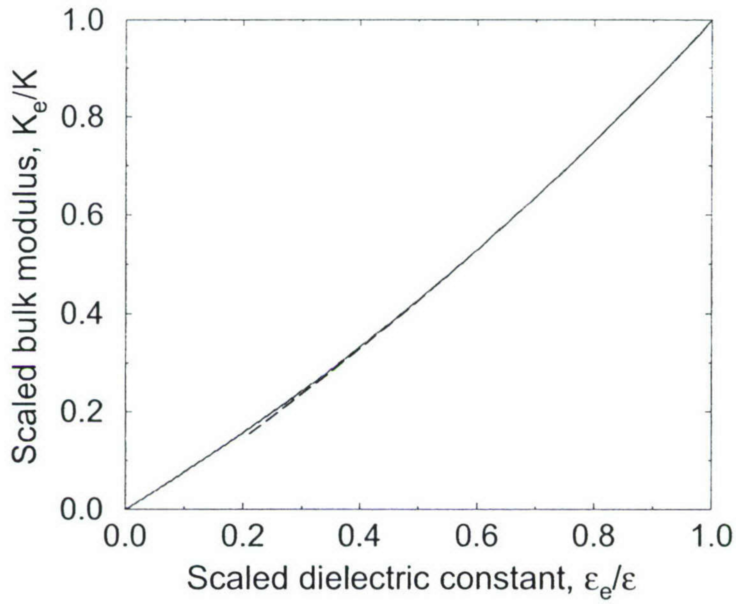

Figure 3: The cross-property upper bound with $\nu = 0.2$ (blue solid line) in the ε_e-K_e plane, which corresponds to an optimal multiscale porous solid. Cross-property relation for identical spherical voids arranged on a FCC lattice (black dashed line) in the ε_e-K_e plane .

and properties have yet to be incorporated, including acoustic, optical, electromagnetic and chemical properties as well as strength behavior.

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